Abstracts of Invited Talks

The Changing Atmosphere 2003

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Earth's atmosphere is not an equilibrium system, but instead is much closer to a photochemical steady state under the influence of the sun. This average steady state can drift over time, at least in part to the direct influences of mankind. Three general effects are considered here; (1) smog created in urban environments (with similar chemistry from biomass burning), (2) depletion of stratospheric ozone by halogenated compounds, allowing more solar ultraviolet radiation to reach Earth's surface, and (3) increasing levels of greenhouse gases, hindering escape of terrestrial infrared radiation, with global warming as a consequence.

Title to be announced

Mostafa A. El-Sayed

Georgia Institute of Technology

Using Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations

William H. Miller

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Semiclassical (SC) theory provides a good description of essentially all quantum effects (interference, tunneling, symmetry effects of identical particles, quantization of bounded motion, etc.) in molecular dynamics; this has been long appreciated and validated by many applications to small molecular systems [cf. Adv. Chem. Phys. **25**, 69-177 (1974)]. Since SC theory is built on the classical trajectories of the dynamical system, it should in principle be possible to use it also to add quantum effects to classical trajectory simulations of *complex* molecular systems (i.e., those with many degrees of freedom), e.g., chemical reactions in solution, clusters, proteins, or any complex environment. The practical implementation of SC theory for complex systems is based on various initial value representations (IVRs), which have recently undergone a re-birth of interest in this regard. This talk reviews the basic idea of the SC-IVR approach and describes a variety of recent applications that have been carried out using it. [For a recent overview, see J. Phys. Chem. A **105**, 2942-2955 (2001).]

Ultrafast Spectroscopy of Small Molecules with Visible and EUV Pulses

Margaret Murnane

University of Colorado, JILA

In this talk, I will discuss the use of shaped, broadband, femtosecond pulses to selectively excite vibrational modes and their overtones at room temperature and pressure. Relatively high spectral selectivity of $15cm^{-1}$ is achieved by carefully designing the shape of the excitation pulse. I will also discuss the use of ultrafast x-ray pulses to monitor charge transfer processes and molecular oscillations on surfaces on femtosecond timescales.

Title to be announced

Yuan T. Lee
Academia Sinica, Taiwan

Overview of Cavity-Enhanced Absorption Spectroscopies

Richard N. Zare
Stanford University, Department of Chemistry

Absorption spectroscopy dates back to the beginning of the last century. It tends to be universal in that almost all matter (dark matter excepted!) absorbs electromagnetic radiation at some frequency, but it also tends to be rather insensitive. Typical absorption measurements cannot see a change in the absorption better than one part in 10,000 or one part in 100,000. This situation has dramatically changed for the better with the introduction of various absorption measurements using optical cavities. This talk will present a review of cavity ring-down spectroscopy and related techniques, emphasizing its use for the detection of absorbing species in gases, liquids, solids, and plasmas.

Spectroscopy with Telescopes: Astrophysical & Atmospheric Puzzles, Laboratory Challenges

Geoffrey A. Blake
Professor of Cosmochemistry & Planetary Science, Professor of Chemistry,
and Deputy Director, Owens Valley Radio Observatory,
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The continuing development and deployment of large aperture telescopes and high performance spectrographs has produced spectra of natural environments with unprecedented sensitivity and resolution. Our understanding of processes as diverse as star formation and ozone destruction has been correspondingly enhanced. This talk will overview recent results from and near-future capabilities in remote sensing at optical through millimeter-wavelengths. Existing and new missions pose severe challenges to laboratory spectroscopy, the bedrock upon which progress is based, and so areas of greatest need in both astrophysics and atmospheric science will be highlighted.